

Access DB# 74082**SEARCH REQUEST FORM**

Scientific and Technical Information Center

Requester's Full Name: BEN SACKLEY Examiner #: \_\_\_\_\_ Date: 8/20/02  
 Art Unit: 1626 Phone Number 305-6889 Serial Number: 07/863,550  
 Mail Box and Bldg/Room Location: CM13E11 Results Format Preferred (circle): PAPER DISK E-MAIL

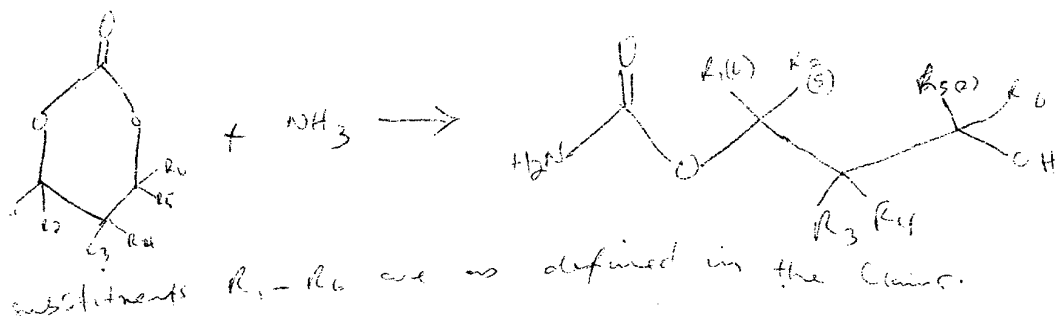
If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Prep. of hydroxyalkyl carbamates from 6-membered cyclic carbamatesInventors (please provide full names): John Clements et al.Earliest Priority Filing Date: 05/23/01

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

**STAFF USE ONLY**Searcher: K. FullerSearcher Phone #: 208-4290

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: 8/27/02Searcher Prep & Review Time: 20

Clerical Prep Time: \_\_\_\_\_

Online Time: 30

PTO-1590 (8-01)

**Type of Search**

NA Sequence (#) \_\_\_\_\_

AA Sequence (#) \_\_\_\_\_

Structure (#) 4

Bibliographic \_\_\_\_\_

Litigation \_\_\_\_\_

Fulltext \_\_\_\_\_

Patent Family \_\_\_\_\_

Other \_\_\_\_\_

**Vendors and cost where applicable**STN ✓

Dialog \_\_\_\_\_

Questel/Orbit \_\_\_\_\_

Dr.Link \_\_\_\_\_

Lexis/Nexis \_\_\_\_\_

Sequence Systems \_\_\_\_\_

WWW/Internet \_\_\_\_\_

Other (specify) \_\_\_\_\_

correct prep. > 2 searches

=> FILE CASRE

FILE 'CASREACT' ENTERED AT 15:19:10 ON 29 AUG 2002  
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FILE CONTENT:1974 - 25 Aug 2002 VOL 137 ISS 8

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> D QUE L15

L13

STR

PRO

15

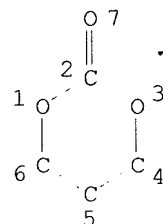
O

~

H2N~C~O~C~C~C~OH  
8 9 10 11 12 13 14

*reactant*

RCT



*Product*

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L15 1 SEA FILE=CASREACT SSS FUL L13 ( 2 REACTIONS)

=> D L15 ALL



L15 ANSWER 1 OF 1 CASREACT COPYRIGHT 2002 ACS

AN 135:92376 CASREACT

TI Preparation of (hydroxyalkyl) carbamates via the ring-opening ammonolysis of 1,3-dioxan-2-ones

IN Clements, John H.; Klein, Howard P.; Marquis, Edward T.; Machac, James R., Jr.

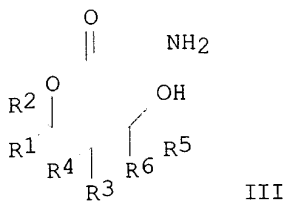
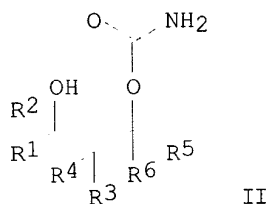
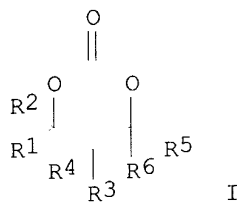
PA Huntsman Petrochemical Corp., USA

*applicants*

KATHLEEN FULLER EIC 1700/LAW LIBRARY 308-4290

SO U.S., 6 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07C269-06  
 NCL 560157000  
 CC 23-20 (Aliphatic Compounds)  
 Section cross-reference(s): 45  
 FAN.CNT 1

|      | PATENT NO.                                                                                                                                                                                                                                                                                                                                                                        | KIND | DATE     | APPLICATION NO. | DATE     |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-----------------|----------|
| PI   | US 6262297                                                                                                                                                                                                                                                                                                                                                                        | B1   | 20010717 | US 2000-669220  | 20000925 |
|      | WO 2002026700                                                                                                                                                                                                                                                                                                                                                                     | A1   | 20020404 | WO 2001-US16053 | 20010518 |
|      | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                 |          |
|      | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG                                                                                                                                                                                        |      |          |                 |          |
|      | US 2002040160                                                                                                                                                                                                                                                                                                                                                                     | A1   | 20020404 | US 2001-863558  | 20010523 |
| PRAI | US 2000-669220                                                                                                                                                                                                                                                                                                                                                                    |      | 20000925 |                 |          |
| OS   | MARPAT 135:92376                                                                                                                                                                                                                                                                                                                                                                  |      |          |                 |          |
| GI   |                                                                                                                                                                                                                                                                                                                                                                                   |      |          |                 |          |



AB When 6-member cyclic carbonate esters [I; H, (un)branched C1-6 alkyl] are subjected to ammonolysis using either anhyd. ammonia or aq. ammonium hydroxide, (hydroxyalkyl) carbamates (II, III) are formed in high yield. Thus, 5-methyl-1,3-dioxan-2-one was reacted with anhyd. ammonia at

55.degree./140 psig, producing 2-methyl-3-hydroxypropyl carbamate in 94.5% yield.

ST dioxanone ring opening ammonolysis prepn hydroxyalkyl carbamate;  
 carboylation ring opening dioxanone prepn hydroxyalkyl carbamate

IT Carbonate esters  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (1,3-dioxan-2-ones; prepn. of (hydroxyalkyl) carbamates via the  
 ring-opening ammonolysis of six-membered cyclic carbonates)

IT Vacuum  
 (in the purifn. of (hydroxyalkyl) carbamates prepd. via the  
 ring-opening ammonolysis of 1,3-dioxan-2-ones)

IT Carbamoylation  
 (ring-opening; prepn. of (hydroxyalkyl) carbamates via the ring-opening  
 ammonolysis of 1,3-dioxan-2-ones)

IT Ammonolysis  
 (ring-opening; prepn. of (hydroxyalkyl) carbamates via the ring-opening  
 ammonolysis of six-membered cyclic carbonates)

IT 1336-21-6, Ammonium hydroxide 7732-18-5, Water, reactions 87831-99-0,  
 5-Methyl-1,3-dioxan-2-one 348110-00-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis  
 of 1,3-dioxan-2-ones)

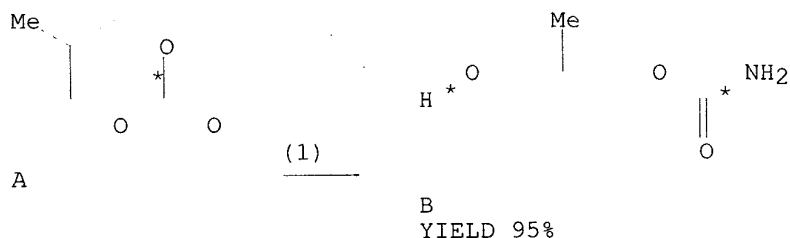
IT 7664-41-7, Ammonia, reactions  
 RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT  
 (Reactant or reagent)  
 (prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis  
 of 1,3-dioxan-2-ones)

IT 17361-58-9P 31521-82-1P 348109-99-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of (hydroxyalkyl) carbamates via the ring-opening ammonolysis  
 of 1,3-dioxan-2-ones)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE

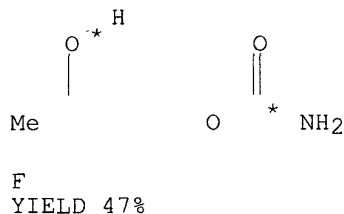
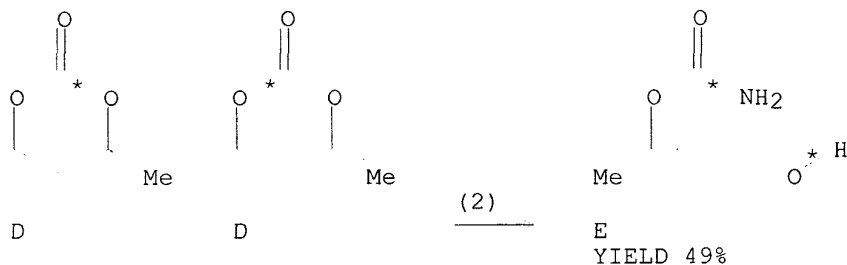
- (1) Angeles; Synthetic Communications 1994, V24(17), P2441 CAPLUS
- (2) Blank; US 4520167 1985 CAPLUS
- (3) Blank; US 4820830 1989 CAPLUS
- (4) Blank; US 5134205 1992 CAPLUS
- (5) Coury; US 4883854 1989 CAPLUS
- (6) Drysdale; US 6020499 2000 CAPLUS
- (7) Forgione; US 5089617 1992 CAPLUS
- (8) Green; International Waterborne, High-Solids, and Powder Coatings Symposium 2000
- (9) Jacobs; US 4897435 1990 CAPLUS
- (10) Parekh; US 4758632 1988 CAPLUS
- (11) Porosoff; US 5102923 1992 CAPLUS
- (12) Reh fuss; US 5605965 1997 CAPLUS

RX(1) OF 2 A ==> B



RX(1) RCT A 87831-99-0  
 RGT C 7664-41-7 NH3  
 PRO B 348109-99-9

RX(2) OF 2 2 D ==> E + F



RX(2) RCT D 17361-58-9  
 RGT C 7664-41-7 NH3  
 PRO E 31521-82-1, F 348110-00-9

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STRUCTURE FILE UPDATES: 27 AUG 2002 HIGHEST RN 445218-02-0  
 DICTIONARY FILE UPDATES: 27 AUG 2002 HIGHEST RN 445218-02-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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 conducting SmartSELECT searches.

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Calculated physical property data is now available. See HELP PROPERTIES  
 for more information. See STNote 27, Searching Properties in the CAS  
 Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> FILE HCAPLUS

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FILE COVERS 1907 - 29 Aug 2002 VOL 137 ISS 9  
FILE LAST UPDATED: 27 Aug 2002 (20020827/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> D QUE

L16 STR

15  
0

H2N- C- O- C- C- C- OH  
8 9 10 11 12 13 14

NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L18 331 SEA FILE=REGISTRY SSS FUL L16  
L19 499 SEA FILE=HCAPLUS ABB=ON L18  
L20 182 SEA FILE=HCAPLUS ABB=ON L19(L) (PREP OR IMF OR SPN)/RL  
L21 5 SEA FILE=HCAPLUS ABB=ON L20 AND (RING?(3A)OPEN? OR RINGOPEN?)  
  
L23 1 SEA FILE=REGISTRY ABB=ON 1336-21-6/RN  
L24 10763 SEA FILE=HCAPLUS ABB=ON L23  
L25 1 SEA FILE=REGISTRY ABB=ON 7664-41-7/RN  
L26 99153 SEA FILE=HCAPLUS ABB=ON L25  
L27 632427 SEA FILE=HCAPLUS ABB=ON L26 OR L24 OR NH3 OR NH4OH OR AMMON?  
L28 27 SEA FILE=HCAPLUS ABB=ON L20 AND L27  
L29 4 SEA FILE=HCAPLUS ABB=ON L28 AND RING?  
L30 2 SEA FILE=HCAPLUS ABB=ON L28 AND ?DIOXAN?  
L31 6 SEA FILE=HCAPLUS ABB=ON L28 AND CYCLIC  
L33 13 SEA FILE=HCAPLUS ABB=ON L21 OR (L29 OR L30 OR L31)

331 structures from  
this query

182  
prep's

=> D L33 ALL 1-13 HITSTR

L33 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 2002:295494 HCAPLUS  
 DN 137:109152  
 TI Studies directed toward the synthesis of the C15-C21 fragment of  
 (-)-discodermolide  
 AU Chakraborty, Tushar K.; Laxman, Pasunoori  
 CS Indian Institute of Chemical Technology, Hyderabad, 500 007, India  
 SO Journal of the Indian Chemical Society (2001), 78(10-12), 543-545  
 CODEN: JICSAH; ISSN: 0019-4522  
 PB Indian Chemical Society  
 DT Journal  
 LA English  
 CC 26-9 (Biomolecules and Their Synthetic Analogs)  
 AB A novel method developed recently for the synthesis of chiral  
 2-methyl-1,3-diols by radical-mediated diastereoselective opening of  
 trisubstituted epoxy alcs. at the more substituted carbon serves as the  
 key step in the studies directed toward the stereoselective synthesis of  
 the C15-C21 fragment of (-)-discodermolide.  
 ST discodermolide stereoselective synthesis  
 IT **Ring opening**  
 (radical, stereoselective; studies directed toward synthesis of C15-C21  
 fragment of (-)-discodermolide)  
 IT Stereoselective synthesis  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT **154335-30-5P, (-)-Discodermolide 443752-38-3P**  
 RL: PNU (Preparation, unclassified); **PREP (Preparation)**  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 72657-23-9 160238-46-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 153775-90-7P 443752-39-4P 443752-40-7P 443752-41-8P 443752-42-9P  
 443752-43-0P 443752-44-1P 443752-45-2P 443752-46-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT  
 (Reactant or reagent)  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 IT 443752-47-4P 443752-48-5P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)  
 RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 RE  
 (1) Balachandran, R; Anticancer Drugs 1998, V9, P67 HCAPLUS  
 (2) Chakraborty, T; Chem Lett 2000, P80 HCAPLUS  
 (3) Chakraborty, T; J Chem Soc, Perkin Trans 1 1997, P1257 HCAPLUS  
 (4) Chakraborty, T; J Indian Chem Soc 1999, V76, P611 HCAPLUS  
 (5) Chakraborty, T; Tetrahedron Lett 1998, V39, P101 HCAPLUS  
 (6) Clark, D; J Org Chem 1993, V58, P5878 HCAPLUS  
 (7) Evans, D; Tetrahedron Lett 1990, V31, P7099 HCAPLUS  
 (8) Evans, D; Tetrahedron Lett 1999, V40, P4461 HCAPLUS  
 (9) Evans, P; Tetrahedron Lett 1993, V34, P8163 HCAPLUS  
 (10) Filla, S; Tetrahedron Lett 1999, V40, P5449 HCAPLUS  
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- (12) Golec, J; Tetrahedron Lett 1993, V34, P8167 HCAPLUS  
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 (15) Harried, S; J Org Chem 1997, V62, P6098 HCAPLUS  
 (16) Hung, D; J Am Chem Soc 1996, V118, P11054 HCAPLUS  
 (17) Kowalski, R; Mol Pharmacol 1997, V52, P613 HCAPLUS  
 (18) Marshall, J; J Org Chem 1998, V63, P7885 HCAPLUS  
 (19) Marshall, J; J Org Chem 1998, V63, P817 HCAPLUS  
 (20) Misske, A; Tetrahedron 1999, V55, P4315 HCAPLUS  
 (21) Miyazawa, M; Chem Lett 1997, P1191 HCAPLUS  
 (22) Miyazawa, M; Chem Lett 1997, P1193 HCAPLUS  
 (23) Nakatsuka, M; J Am Chem Soc 1990, V112, P5583 HCAPLUS  
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 (25) Paterson, I; Angew Chem, Int Ed 2000, V39, P377  
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 (29) Sajiki, H; Tetrahedron Lett 1995, V36, P3456  
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 (33) Yang, G; Tetrahedron Lett 1994, V35, P1313 HCAPLUS  
 (34) Yang, G; Tetrahedron Lett 1994, V35, P2503 HCAPLUS

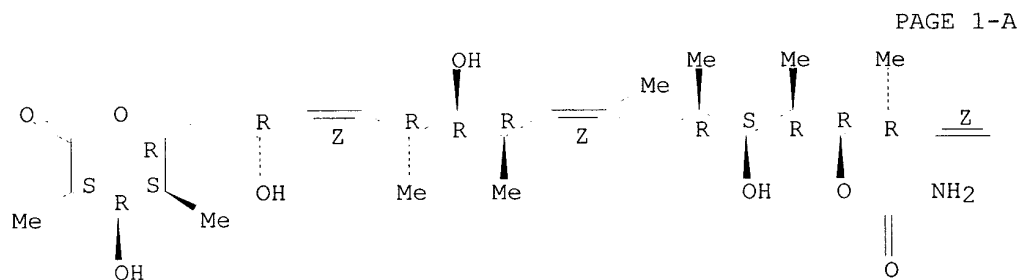
IT 154335-30-5P, (-)-Discodermolide

RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (studies directed toward synthesis of C15-C21 fragment of  
 (-)-discodermolide)

RN 154335-30-5 HCAPLUS

CN 2H-Pyran-2-one, 6-[(2R,3Z,5R,6R,7R,8Z,11R,12S,13R,14R,15R,16Z)-14-  
 [(aminocarbonyl)oxy]-2,6,12-trihydroxy-5,7,9,11,13,15-hexamethyl-3,8,16,18-  
 nonadecatetraenyl]tetrahydro-4-hydroxy-3,5-dimethyl-, (3S,4R,5S,6R)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



CH<sub>2</sub>

L33 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 2001:521946 HCAPLUS

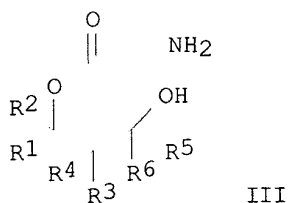
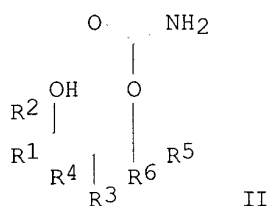
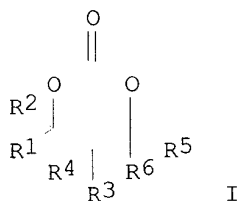
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DN 135:92376  
 TI Preparation of (hydroxyalkyl) carbamates via the ring-  
 opening ammonolysis of 1,3-dioxan-2-ones  
 IN Clements, John H.; Klein, Howard P.; Marquis, Edward T.; Machac, James R.,  
 Jr.  
 PA Huntsman Petrochemical Corp., USA  
 SO U.S., 6 pp. *applicants*  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 IC ICM C07C269-06  
 NCL 560157000  
 CC 23-20 (Aliphatic Compounds)  
 Section cross-reference(s): 45

FAN.CNT 1

|      | PATENT NO.                                                                                                                                                                                                                                                                                                                                                                        | KIND | DATE     | APPLICATION NO. | DATE     |
|------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-----------------|----------|
| PI   | US 6262297                                                                                                                                                                                                                                                                                                                                                                        | B1   | 20010717 | US 2000-669220  | 20000925 |
|      | WO 2002026700                                                                                                                                                                                                                                                                                                                                                                     | A1   | 20020404 | WO 2001-US16053 | 20010518 |
|      | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM |      |          |                 |          |
|      | RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG                                                                                                                                                                                        |      |          |                 |          |
|      | US 2002040160                                                                                                                                                                                                                                                                                                                                                                     | A1   | 20020404 | US 2001-863558  | 20010523 |
| PRAI | US 2000-669220                                                                                                                                                                                                                                                                                                                                                                    | A    | 20000925 |                 |          |
| OS   | CASREACT 135:92376; MARPAT 135:92376                                                                                                                                                                                                                                                                                                                                              |      |          |                 |          |
| GI   |                                                                                                                                                                                                                                                                                                                                                                                   |      |          |                 |          |



AB When 6-member **cyclic** carbonate esters [I; H, (un)branched C1-6 alkyl] are subjected to **ammonolysis** using either anhyd. **ammonia** or aq. **ammonium** hydroxide, (hydroxyalkyl) carbamates (II, III) are formed in high yield. Thus; 5-methyl-1,3-**dioxan-2-one** was reacted with anhyd. **ammonia** at 55.degree./140 psig, producing 2-methyl-3-hydroxypropyl carbamate in 94.5% yield.

ST **dioxanone ring opening ammonolysis**  
prepn hydroxyalkyl carbamate; carbonylation **ring opening**  
**dioxanone** prepn hydroxyalkyl carbamate

IT Carbonate esters  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(1,3-**dioxan-2-ones**; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of six-membered **cyclic** carbonates)

IT Vacuum  
(in the purifn. of (hydroxyalkyl) carbamates prepd. via the **ring-opening ammonolysis** of 1,3-**dioxan-2-ones**)

IT Carbamoylation  
(**ring-opening**; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-**dioxan-2-ones**)

IT **Ammonolysis**  
(**ring-opening**; prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of six-membered **cyclic** carbonates)

IT **1336-21-6, Ammonium** hydroxide 7732-18-5, Water, reactions 87831-99-0, 5-Methyl-1,3-**dioxan-2-one** 348110-00-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-**dioxan-2-ones**)

IT **7664-41-7, Ammonia**, reactions  
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT (Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-**dioxan-2-ones**)

IT 17361-58-9P 31521-82-1P 348109-99-9P  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(prepn. of (hydroxyalkyl) carbamates via the **ring-opening ammonolysis** of 1,3-**dioxan-2-ones**)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE  
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(2) Blank; US 4520167 1985 HCAPLUS  
(3) Blank; US 4820830 1989 HCAPLUS  
(4) Blank; US 5134205 1992 HCAPLUS  
(5) Coury; US 4883854 1989 HCAPLUS  
(6) Drysdale; US 6020499 2000 HCAPLUS  
(7) Forgione; US 5089617 1992 HCAPLUS  
(8) Green; International Waterborne, High-Solids, and Powder Coatings Symposium 2000  
(9) Jacobs; US 4897435 1990 HCAPLUS  
(10) Parekh; US 4758632 1988 HCAPLUS  
(11) Porosoff; US 5102923 1992 HCAPLUS  
(12) Rehfuss; US 5605965 1997 HCAPLUS

IT **1336-21-6, Ammonium** hydroxide  
RL: RCT (Reactant); RACT (Reactant or reagent)

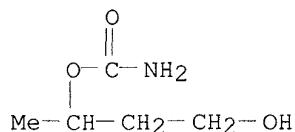
(prepn. of (hydroxyalkyl) carbamates via the ring-  
opening ammonolysis of 1,3-dioxan-2-ones)  
RN 1336-21-6 HCAPLUS  
CN Ammonium hydroxide ((NH4)(OH)) (9CI) (CA INDEX NAME)

H4N-OH

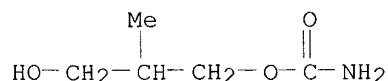
IT 7664-41-7, Ammonia, reactions  
RL: RCT (Reactant); REM (Removal or disposal); PROC (Process); RACT  
(Reactant or reagent)  
(prepn. of (hydroxyalkyl) carbamates via the ring-  
opening ammonolysis of 1,3-dioxan-2-ones)  
RN 7664-41-7 HCAPLUS  
CN Ammonia (8CI, 9CI) (CA INDEX NAME)

NH3

IT 31521-82-1P 348109-99-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of (hydroxyalkyl) carbamates via the ring-  
opening ammonolysis of 1,3-dioxan-2-ones)  
RN 31521-82-1 HCAPLUS  
CN 1,3-Butanediol, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 348109-99-9 HCAPLUS  
CN 1,3-Propanediol, 2-methyl-, monocarbamate (9CI) (CA INDEX NAME)



L33 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
AN 1999:566027 HCAPLUS  
DN 131:184942  
TI Preparation of 3-(5-isoxazolyl)- or 3-phenylpropylamine derivatives as  
central muscle relaxants  
IN Matsui, Takeaki; Tanaka, Yuichiro; Inoue, Masaki; Etoh, Shugo; Noda,  
Masatoshi; Yabuki, Tetsuaki; Toga, Tetsuo; Amagishi, Hiroaki; Hayakawa,  
Maki; Tanaka, Chikage; Matsumura, Yumi  
PA Maruho Kabushikikaisha, Japan  
SO PCT Int. Appl., 66 pp.  
CODEN: PIXXD2  
DT Patent  
LA Japanese  
IC ICM C07D211-14

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ICS C07D261-08; C07D277-28; C07D295-092; C07D307-52; C07D307-81;  
C07D333-20; C07D333-58; A61K031-40; A61K031-42; A61K031-425;  
A61K031-445; A61K031-535; A61K031-55

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

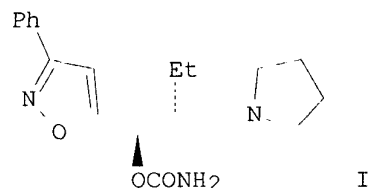
FAN.CNT 1

|    | PATENT NO.                                                                 | KIND | DATE     | APPLICATION NO. | DATE     |
|----|----------------------------------------------------------------------------|------|----------|-----------------|----------|
| PI | WO 9943656                                                                 | A1   | 19990902 | WO 1999-JP759   | 19990219 |
|    | W: CN, JP, KR, US                                                          |      |          |                 |          |
|    | RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |          |                 |          |

PRAI JP 1998-43998 19980225

OS MARPAT 131:184942

GI



AB Propylamine derivs. represented by formula  $ACH(O_2CNHR_5)CR_1R_2CH_2NR_3R_4$  and salts thereof (wherein A is substituted aryl or optionally substituted heteroaryl; R<sub>1</sub> and R<sub>2</sub> are the same or different lower alkyls, or one of R<sub>1</sub> and R<sub>2</sub> is hydrogen and the other is lower alkyl, lower alkoxy, aryl, aralkyl, or lower alkoxy- or lower alkylthio-substituted lower alkyl; one of R<sub>3</sub> and R<sub>4</sub> is hydrogen or lower alkyl and the other is lower cycloalkyl, or R<sub>3</sub> or R<sub>4</sub> are the same or different lower alkyls or are bonded to each other to form a **ring** which contains one or more nitrogen or oxygen atoms and is optionally substituted by lower alkyl, lower alkanoyl, or aralkyl; and R<sub>5</sub> is hydrogen, lower alkyl, or aryl) are prep'd. These compds. are useful as central muscle relaxants or for the treatment of urination disorders. Thus, (1R,2R)-5-[1-hydroxy-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole was condensed with Ph chlorocarbonate in pyridine/CH<sub>2</sub>Cl<sub>2</sub> at room temp. for 2 h and the amidated with NH<sub>3</sub> in 2-propanol at room temp. for 4 h to give, after salt formation with oxalic acid, (1R,2R)-5-[1-(carbamoyloxy)-2-(1-pyrrolidinylmethyl)butyl]-3-phenylisoxazole [I.(CO<sub>2</sub>H)<sub>2</sub>]. I.(CO<sub>2</sub>H)<sub>2</sub> at 4.0 mg/kg p.o relaxed 84.7% decerebrate rigidity in rats.

ST isoxazolylpropylamine prepn central muscle relaxant; urination disorder treatment carbamoyloxypyrrolidinylmethylbutylphenylisoxazole; phenylisoxazole carbamoyloxy pyrrolidinylmethyl butyl prepn; phenylpropylamine prepn central muscle relaxant

IT Muscle relaxants  
(central; prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

IT Micturition  
(disorder; prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

|    |              |              |              |              |              |
|----|--------------|--------------|--------------|--------------|--------------|
| IT | 240123-98-2P | 240124-01-0P | 240124-04-3P | 240124-08-7P | 240124-12-3P |
|    | 240124-14-5P | 240124-16-7P | 240124-17-8P | 240124-20-3P | 240124-22-5P |
|    | 240124-23-6P | 240124-25-8P | 240124-26-9P | 240124-29-2P | 240124-31-6P |
|    | 240124-32-7P | 240124-33-8P | 240124-34-9P | 240124-55-4P | 240124-56-5P |
|    | 240124-57-6P | 240124-58-7P | 240124-61-2P | 240404-84-6P |              |

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

IT 75-04-7, Ethylamine, reactions 98-59-9, p-Toluenesulfonyl chloride 103-71-9, Phenyl isocyanate, reactions 123-75-1, Pyrrolidine, reactions 141-75-3, n-Butyryl chloride 17016-83-0, (S)-4-Isopropylloxazolidin-2-one 64840-90-0 72418-40-7 95530-58-8, (R)-4-Isopropylloxazolidin-2-one 145588-94-9 166740-28-9 166740-30-3 166740-32-5 179077-80-6 240124-65-6 240124-67-8 240124-68-9 240124-69-0 240124-70-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

IT 157796-13-9P 240124-27-0P 240124-28-1P 240124-30-5P 240124-35-0P 240124-36-1P 240124-37-2P **240124-38-3P** 240124-39-4P 240124-40-7P 240124-41-8P 240124-42-9P **240124-43-0P** 240124-44-1P 240124-45-2P 240124-46-3P 240124-47-4P **240124-48-5P** 240124-49-6P 240124-50-9P 240124-51-0P 240124-52-1P **240124-53-2P** 240124-54-3P 240124-59-8P 240124-60-1P 240124-62-3P 240124-63-4P 240124-64-5P

RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**

**(Preparation); RACT (Reactant or reagent)**

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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- (2) Bayer Ag; DE 3019496 A HCAPLUS
- (3) Bayer Ag; EP 40740 A HCAPLUS
- (4) Bayer Ag; US 4495184 A HCAPLUS
- (5) Bayer Ag; JP 5716841 A 1982

IT **240124-38-3P 240124-43-0P 240124-48-5P**

**240124-53-2P**

RL: RCT (Reactant); **SPN (Synthetic preparation); PREP**

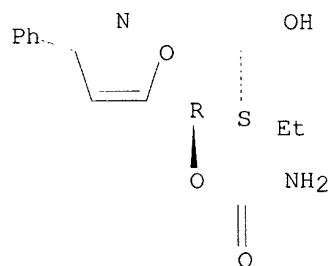
**(Preparation); RACT (Reactant or reagent)**

(prepn. of (isoxazolyl)propylamine derivs. as central muscle relaxants and for treatment of urination disorders)

RN 240124-38-3 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1R,2S)- (9CI) (CA INDEX NAME)

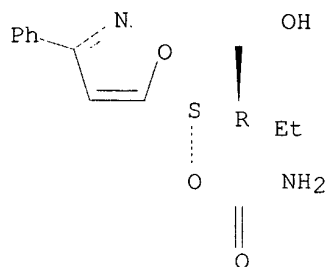
Absolute stereochemistry. Rotation (+).



RN 240124-43-0 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1S,2R)- (9CI) (CA INDEX NAME)

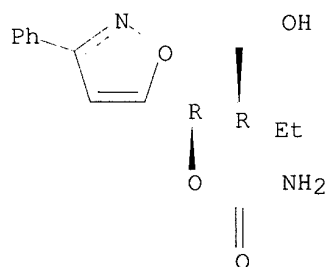
Absolute stereochemistry. Rotation (-).



RN 240124-48-5 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1R,2R)-  
(9CI) (CA INDEX NAME)

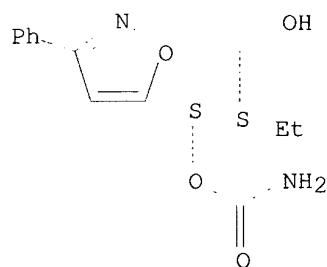
Absolute stereochemistry. Rotation (+).



RN 240124-53-2 HCAPLUS

CN 1,3-Propanediol, 2-ethyl-1-(3-phenyl-5-isoxazolyl)-, 1-carbamate, (1S,2S)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L33 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1999:286766 HCAPLUS

DN 131:129813

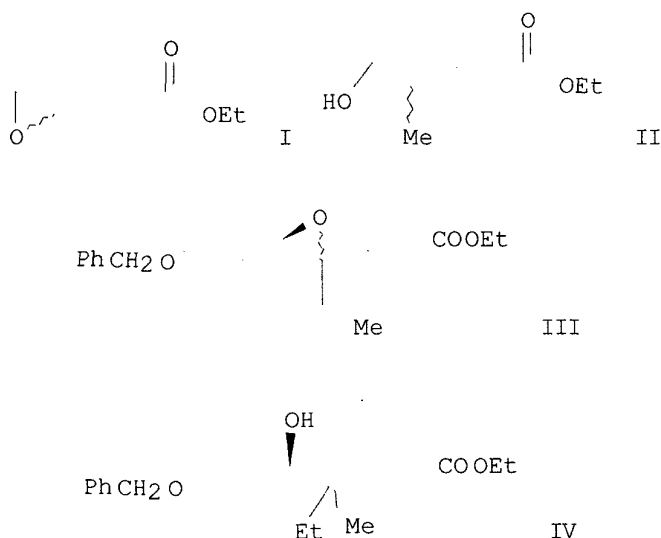
TI Natural product synthesis based on the stereospecific acyclic  
stereocontrolAU Miyazawa, Masahiro; Maruyama, Kimiyuki; Sasaki, Shinobu; Ohnuma, Satoshi;  
Ishibashi, Naoki; Sasaki, Minoru; Miyashita, Masaaki

CS Graduate School of Science, Hokkaido University, Japan

SO Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 211-216

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CODEN: TYKYDS  
 PB Nippon Kagakkai  
 DT Journal  
 LA Japanese  
 CC 26-9 (Biomolecules and Their Synthetic Analogs)  
 GI



AB The authors recently developed a novel acyclic stereocontrol based on the stereospecific methylation of .gamma.,.delta.-epoxy acrylates with trimethylaluminum in the presence of water by which both anti and syn compds. can be highly stereoselectively synthesized from trans- and cis-.gamma.,.delta.-epoxy acrylates, resp. The authors report here stereospecific internal alkylation of terminal epoxides and stereospecific construction of asym. quaternary carbons via .gamma.,.delta.-epoxy acrylates. The authors also report synthetic studies toward total synthesis of a marine natural product discodermolide and epothilone based on the above methodologies. Regio- and stereoselective internal alkylation of terminal epoxides has little been known. The authors designed such a reaction using .gamma.,.delta.-epoxy acrylates with trimethylaluminum. The reaction of terminal .gamma.,.delta.-epoxy acrylates (S)- and (R)-I, easily prepd. from D-mannitol, with excess trimethylaluminum in the presence of water proceeded regiospecifically at the .gamma.-position to give (R)- and (S)-II, as the sole product, resp., with maintenance of optical integrity. Regarding stereospecific construction of asym. quaternary carbons via .gamma.-Alkyl-.gamma.,.delta.-epoxy acrylates, the authors found that the reaction of .gamma.-alkyl-.gamma.,.delta.-epoxy acrylates with trialkylaluminum and water occurs regio- and stereo-specifically at the .gamma.-position as well yielding an asym. quaternary carbon. Thus, treatment of (4R)- and (4S)-III with excess trimethylaluminum in the presence of water gave (4R)- and (4S)-IV as a single product, resp., in which a Me group was stereospecifically introduced at the .gamma.-position with net inversion of configuration. Regarding synthetic studies on discodermolide and epothilone, the authors set out synthesis of discodermolide having potent immunosuppressive activity based on the above stereospecific acyclic stereocontrol. Discodermolide was divided into three segments in which

the segment B having three contiguous chiral centers and the segment C possessing five chiral centers have been highly stereoselectively synthesized. Stereoselective synthesis of the C1-C9 segment of epothilone having potent anticancer activity was also carried out in which five asym. centers was highly stereoselectively constructed by repeating the above methylation reaction.

ST stereospecific acyclic stereocontrol natural product synthesis

IT Natural products

RL: SPN (Synthetic preparation); PREP (Preparation)  
(natural product synthesis based on stereospecific acyclic  
stereocontrol)

IT Alkylation

(stereoselective; natural product synthesis based on stereospecific acyclic stereocontrol)

IT 191275-35-1 191275-36-2 234769-47-2 234769-48-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(natural product synthesis based on stereospecific acyclic  
stereocontrol)

IT **127943-53-7P**, Discodermolide 152044-53-6DP, Epothilone a,  
analogs 191275-37-3P 191275-38-4P 234769-49-4P 234769-50-7P

RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(natural product synthesis based on stereospecific acyclic  
stereocontrol)

IT 75-24-1, Trimethyl aluminum

RL: RCT (Reactant); RACT (Reactant or reagent)  
(stereospecific alkylation and epoxide **ring opening**  
by)

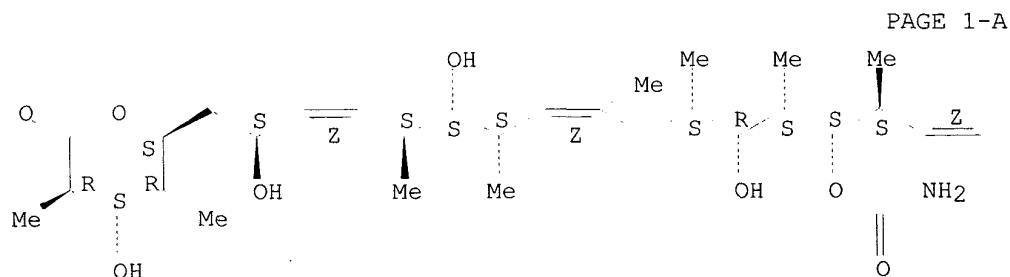
IT 127943-53-7P, Discodermolide

RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(natural product synthesis based on stereospecific acyclic  
stereocontrol)

RN 127943-53-7 HCAPLUS

CN 2H-Pyran-2-one, 6-[(2S,3Z,5S,6S,7S,8Z,11S,12R,13S,14S,15S,16Z)-14-  
[(aminocarbonyl)oxy]-2,6,12-trihydroxy-5,7,9,11,13,15-hexamethyl-3,8,16,18-  
nonadecatetraenyl]tetrahydro-4-hydroxy-3,5-dimethyl-, (3R,4S,5R,6S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



PAGE 1-B

 $\text{CH}_2$



L33 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
AN 1999:202358 HCAPLUS  
DN 130:267674  
TI Total Synthesis of (+)-Polyoxin J  
AU Ghosh, Arun K.; Wang, Yong  
CS Department of Chemistry, University of Illinois at Chicago, Chicago, IL, 60607, USA  
SO Journal of Organic Chemistry (1999), 64(8), 2789-2795  
CODEN: JOCEAH; ISSN: 0022-3263  
PB American Chemical Society  
DT Journal  
LA English  
CC 33-7 (Carbohydrates)  
OS CASREACT 130:267674  
AB Stereoselective total synthesis of (+)-polyoxin J is described. The synthesis was achieved in a convergent manner by coupling protected thymine polyoxin C and 5-O-carbamoyl polyoxamic acid and subsequent removal of the protecting groups. The key steps of the synthesis of protected thymine polyoxin C involved the stereoselective electrophilic epoxidn. of an E-allyl alc. derived from isopropylidene D-ribose deriv., followed by regioselective epoxide opening of the syn-epoxide and conversion of resulting azido diol to protected thymine polyoxin C. Protected polyoxamic acid was synthesized stereoselectively by utilizing Sharpless epoxidn. of a tartrate-derived allylic alc. followed by a regioselective epoxide **ring opening** with diisopropoxytitanium diazide.  
ST thymine polyoxin C stereoselective epoxidn regioselective epoxide opening; polyoxin J stereoselective total synthesis  
IT **Ring opening**  
(regioselective; total synthesis of (+)-polyoxin J)  
IT Epoxidation  
(stereoselective; total synthesis of (+)-polyoxin J)  
IT 65-71-4, Thymine 108818-00-4 131121-18-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(total synthesis of (+)-polyoxin J)  
IT 58934-84-2P 90661-54-4P 105309-43-1P 127257-35-6P 127646-34-8P  
130193-61-2P 143833-90-3P 155023-01-1P 213973-65-0P 222400-52-4P  
222400-53-5P 222400-54-6P 222400-56-8P 222400-57-9P 222403-61-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(total synthesis of (+)-polyoxin J)  
IT **22976-89-2P** 143833-91-4P 222400-55-7P  
RL: **SPN (Synthetic preparation); PREP (Preparation)**  
(total synthesis of (+)-polyoxin J)  
RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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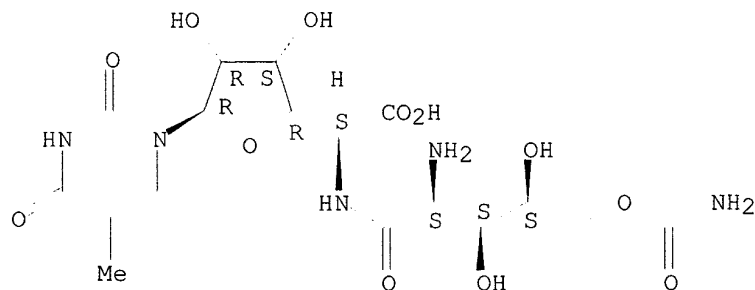
IT 22976-89-2P

RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (total synthesis of (+)-polyoxin J)

RN 22976-89-2 HCAPLUS

CN .beta.-D-Allofuranuronic acid, 5-[[2-amino-5-O-(aminocarbonyl)-2-deoxy-L-xylonoyl]amino]-1,5-dideoxy-1-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L33 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1997:421294 HCAPLUS

DN 127:34005

TI Novel sulfamate compounds containing an N-substituted carbamoyl group, useful as CNS drugs, and method for preparing them

IN Choi, Yong Moon; Han, Dong Il; Kim, Hyung Cheol

PA Yukong Limited, S. Korea

SO PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07C307-02

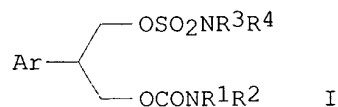
ICS A61K031-27

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

FAN.CNT 3

|      | PATENT NO.                                                             | KIND | DATE     | APPLICATION NO. | DATE     |
|------|------------------------------------------------------------------------|------|----------|-----------------|----------|
| PI   | WO 9716418                                                             | A1   | 19970509 | WO 1996-KR190   | 19961101 |
|      | W: CA, CN, JP                                                          |      |          |                 |          |
|      | RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |          |                 |          |
|      | CA 2209229                                                             | AA   | 19970509 | CA 1996-2209229 | 19961101 |
|      | EP 801642                                                              | A1   | 19971022 | EP 1996-935567  | 19961101 |
|      | EP 801642                                                              | B1   | 20001220 |                 |          |
|      | R: BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE              |      |          |                 |          |
|      | CN 1173864                                                             | A    | 19980218 | CN 1996-191830  | 19961101 |
|      | CN 1077570                                                             | B    | 20020109 |                 |          |
|      | JP 10512591                                                            | T2   | 19981202 | JP 1996-517235  | 19961101 |
|      | ES 2154840                                                             | T3   | 20010416 | ES 1996-935567  | 19961101 |
| PRAI | KR 1995-39456                                                          | A    | 19951102 |                 |          |
|      | KR 1996-49052                                                          | A    | 19961028 |                 |          |
|      | WO 1996-KR190                                                          | W    | 19961101 |                 |          |
| OS   | MARPAT 127:34005                                                       |      |          |                 |          |
| GI   |                                                                        |      |          |                 |          |



AB Novel sulfamate compds. contg. an N-substituted carbamoyl group are disclosed, specifically I [Ar = (un)substituted Ph; R1, R2, R3, R4 = H,

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alkyl, cycloalkyl, aryl; or NR1R2 and/or NR3R4 may form 3- to 7-membered aliph. **cyclic** structure(s) with another N or O atom], including both their racemates and (R)- and (S)-optical isomers. I are useful for the prophylaxis and treatment of disorders of the central nervous system, esp. nervous myalgia, epilepsy, and minimal brain dysfunction (no data). For instance, reaction of AcOCH2CHPhCH2OH with carbonyldiimidazole in CH2Cl2 and then with aq. NH3 gave 95% AcOCH2CHPhCH2OCONH2. This compd. was deacetylated with KCN in MeOH (88%), and the resultant alc. was sulfamoylated with ClSO2NH2 in pyridine (85%), to give title compd. H2NSO2OCH2CHPhCH2OCONH2. A variety of substituted I, including (R)- and (S)-isomers, were prepd. by this and other methods.

ST phenylpropanediol carbamate sulfamate prepn CNS drug; antiepileptic propanediol carbamate sulfamate prepn

IT Muscle, disease  
(myalgia, treatment; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT Cytoprotective agents  
(neuroprotectants; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT Anticonvulsants  
Nervous system agents  
(prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT Brain, disease  
(stroke, treatment; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT Brain  
(treatment of minimal dysfunction; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT **25451-53-0P 171433-01-5P 171433-04-8P**  
 178759-04-1P 178759-44-9P 190589-95-8P 190589-96-9P 190589-97-0P  
 190589-98-1P 190589-99-2P 190590-00-2P 190590-01-3P 190590-03-5P  
 190590-04-6P 190590-05-7P 190590-06-8P 190590-07-9P 190590-08-0P  
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 190590-39-7P 190590-47-7P 190590-48-8P 190590-49-9P 190590-50-2P  
 190590-51-3P 190590-52-4P 190590-53-5P 190590-54-6P 190590-55-7P  
 190590-56-8P 190590-57-9P 190590-58-0P  
 RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation);** RACT (Reactant or reagent)  
 (intermediate; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT 190590-09-1P 190590-10-4P 190590-11-5P 190590-12-6P 190590-13-7P  
 190590-14-8P 190590-15-9P 190590-18-2P 190590-31-9P 190590-32-0P  
 190590-33-1P 190590-34-2P 190590-35-3P 190590-36-4P 190590-37-5P  
 190590-41-1P 190590-42-2P 190590-43-3P 190590-44-4P 190590-45-5P  
 190590-46-6P 190590-59-1P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

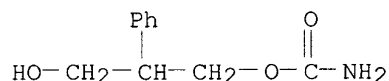
IT 74-89-5, Methylamine, reactions 75-31-0, Isopropylamine, reactions 103-71-9, Phenyl isocyanate, reactions 110-91-8, Morpholine, reactions 124-40-3, Dimethylamine, reactions 530-62-1 765-30-0, Cyclopropylamine 7778-42-9, Sulfamoyl chloride 110230-69-8 110270-51-4 126986-28-5  
 190590-60-4 190590-61-5 190897-00-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (starting material; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

IT **25451-53-0P 171433-01-5P 171433-04-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; prepn. of phenylpropanediol carbamate sulfamate compds. as CNS agents)

RN 25451-53-0 HCAPLUS

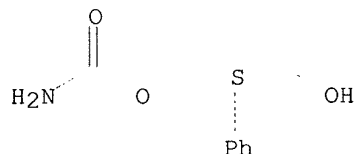
CN 1,3-Propanediol, 2-phenyl-, monocarbamate (8CI, 9CI) (CA INDEX NAME)



RN 171433-01-5 HCAPLUS

CN 1,3-Propanediol, 2-phenyl-, monocarbamate, (2S)- (9CI) (CA INDEX NAME)

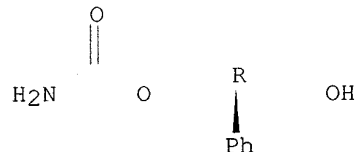
Absolute stereochemistry.



RN 171433-04-8 HCAPLUS

CN 1,3-Propanediol, 2-phenyl-, monocarbamate, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1992:570572 HCAPLUS

DN 117:170572

TI Unique carbamation of 2-(2-pyridyl)-1,3-propanediol by phosgenation followed by **ammonolysis**

AU Choi, Yong Moon; Rosso, Victor; Kucharczyk, Norbert; Sofia, R. Duane

CS Wallace Lab., Cranbury, NJ, 08512, USA

SO J. Org. Chem. (1992), 57(21), 5764-6

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

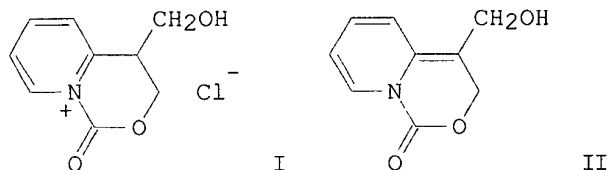
LA English

CC 22-4 (Physical Organic Chemistry)

Section cross-reference(s): 27

OS CASREACT 117:170572

GI



- AB The unique phosgenation between 2-(2-pyridyl)-1,3-propanediol and ClCOCl in pyridine or THF contg. Et3N makes available intramol. **cyclic**, 1H-pyrido[1,2-c][1,3]-3,4-dihydro-4-(hydroxymethyl)-1-oxooxazinium chloride salt (I) which is characterized. **NH3** reacts with I to give RCH(CH2OH)CH2O2CNH2 (R = 2-pyridyl). The combined reactions (phosgenation and **ammonolysis**), thus, are systematically studied and compared at 0.degree., -30.degree., and -70.degree.. The unexpected products, the deprotonated second **cyclic** intermediate, 1H,3H-pyrido[1,2-c][1,3]oxazin-4-hydroxymethyl-1-one (II) and 2-(2-pyridyl)-3-hydroxypropene, are derived from the salt-like intermediate by .alpha.-proton abstraction. At an appropriate lower temp. the carbamation successfully competes with the .alpha.-proton abstraction.
- ST carbamation pyridylpropanediol mechanism; phosgenation **ammonolysis** pyridylpropanediol; pyridooxazinium chloride **ammonolysis**
- IT **Ring cleavage**  
(of pyridodihydro(hydroxymethyl)oxooxazinium chloride by **ammonia**, deprotonation vs.)
- IT Cyclocondensation reaction  
(of pyridylpropanediol with phosgene)
- IT **Ammonolysis**  
(phosgenation and, of pyridylpropanediol, mechanism of)
- IT Protonation and Proton transfer reaction  
(deprotonation, of pyridodihydro(hydroxymethyl)oxooxazinium chloride by **ammonia** or amines, **ring** cleavage and)
- IT Acylation  
(phosgenation, **ammonolysis** and, for carbamation of pyridylpropanediol, mechanism of)
- IT **7664-41-7**  
RL: RCT (Reactant)  
(**ammonolysis**, phosgenation and, of pyridylpropanediol, mechanism of)
- IT 49745-42-8, 2-(2-Pyridyl)-1,3-propanediol  
RL: RCT (Reactant)  
(carbamation of, with phosgene in presence of triethylamine, mechanism of)
- IT 75-44-5, Phosgene  
RL: RCT (Reactant)  
(carbamation with, of pyridylpropanediol)
- IT 137518-88-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and **ring** cleavage and deprotonation of, mechanism of)
- IT 554-68-7P, Triethylamine hydrochloride 58379-60-5P 137094-10-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)
- IT **86199-37-3P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, mechanism of)
- IT 12408-02-5  
RL: RCT (Reactant)

(protonation and Proton transfer reaction, deprotonation, of pyridodihydro(hydroxymethyl)oxooxazinium chloride by ammonia or amines, ring cleavage and)

IT 7664-41-7

RL: RCT (Reactant)

(ammonolysis, phosgenation and, of pyridylpropanediol, mechanism of)

RN 7664-41-7 HCAPLUS

CN Ammonia (8CI, 9CI) (CA INDEX NAME)

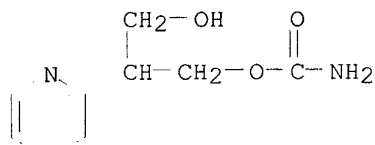
NH<sub>3</sub>

IT 86199-37-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, mechanism of)

RN 86199-37-3 HCAPLUS

CN 1,3-Propanediol, 2-(2-pyridinyl)-, monocarbamate (ester) (9CI) (CA INDEX NAME)



L33 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1989:439851 HCAPLUS

DN 111:39851

TI Preparation and testing of bactericidal .alpha.-hydroxy-.beta.-lysine derivatives

IN Masuya, Hiromoto; Harada, Setsuo; Natsugari, Hideaki

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 120 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07C123-00

ICS C07C125-065; C07C103-66; C07C109-08; C07D295-12; C07D295-18;  
C07F007-18; A61K031-155; A61K031-27; A61K031-16; A61K031-195

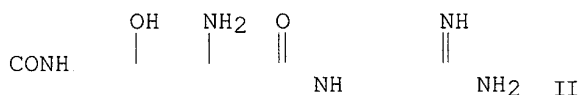
CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 16

FAN.CNT 1

|      | PATENT NO.                                            | KIND | DATE     | APPLICATION NO. | DATE     |
|------|-------------------------------------------------------|------|----------|-----------------|----------|
| PI   | EP 271829                                             | A2   | 19880622 | EP 1987-118314  | 19871210 |
|      | EP 271829                                             | A3   | 19890726 |                 |          |
|      | EP 271829                                             | B1   | 19930825 |                 |          |
|      | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE |      |          |                 |          |
|      | JP 63277652                                           | A2   | 19881115 | JP 1987-306382  | 19871202 |
|      | AT 93513                                              | E    | 19930915 | AT 1987-118314  | 19871210 |
| PRAI | JP 1986-294432                                        |      | 19861210 |                 |          |
|      | JP 1987-306382                                        |      | 19871202 |                 |          |
|      | EP 1987-118314                                        |      | 19871210 |                 |          |
| OS   | MARPAT 111:39851                                      |      |          |                 |          |

GI



- AB R1CHR2CH(OR3)CH2CHR4CH2COR5 [I; R1, R4 = (substituted) amino; R2 = H, (substituted) alkyl; R3 = H, protecting group; R5 = OH, amino, etc.] useful as antibacterials, were prepd. H2NCH2CH(OH)CH2CH(NHBOC)CH2CONHCH2C H2C(:NH)NH2.2HCl (BOC = Me3CO2C) in DMF was acylated by crotonic acid in the presence of Et3N/DCC/hydroxybenzotriazole and the product was deprotected with CF3CO2H to give .delta.-hydroxy-.beta.-lysine deriv. II. Several II had MIC's of 100 .mu.g/mL against Streptococcus aureus 308A-I and ED50's in mice of 4.42-25 mg/kg s.c.
- ST hydroxybetalysine deriv prepn antibacterial; bactericide  
alkenylcarbonylhydroxybetalysine; lysine hydroxybeta prepn antibacterial;  
amino acid deriv hydroxylysine prepn bactericide
- IT Yeast  
(chiral redn. by, of ketoaminobutyrate deriv.)
- IT Pseudomonas acidovorans  
(deacylation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT Pseudomonas fluorescens  
(hydroxylysine deriv. manuf. with, in prepn. of bactericide)
- IT Bactericides, Disinfectants, and Antiseptics  
(hydroxylysine derivs.)
- IT Asymmetric synthesis and induction  
(of hydroxylysine bactericides)
- IT Amino acids, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(derivs., hydroxylysine, prepn. of, as bactericides)
- IT 501-53-1, Carbobenzoxy chloride 17341-93-4, 2,2,2-Trichloroethoxycarbonyl chloride  
RL: RCT (Reactant)  
(acylation by, of amino lactone deriv., in prepn. of bactericide)
- IT 98-88-4, Benzoyl chloride 501-53-1, Benzyloxycarbonyl chloride  
2614-88-2 3724-65-0, 2-Butenoic acid  
RL: RCT (Reactant)  
(acylation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 110-44-1, Sorbic acid 91028-39-6  
RL: RCT (Reactant)  
(acylation by, of .beta.-lysine deriv., in prepn. of bactericide)
- IT 60099-09-4, Benzyl formimidate hydrochloride 113904-16-8  
RL: RCT (Reactant)  
(amidation by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 82353-56-8  
RL: RCT (Reactant)  
(chiral cyclocondensation of, with silyloxydiene deriv.)
- IT 38330-80-2, Potassium monomethyl malonate  
RL: RCT (Reactant)  
(condensation of, with alanine deriv.)
- IT 7803-57-8, Hydrazine hydrate 51127-12-9 60099-09-4, Benzyl formimidate hydrochloride 82102-87-2 107819-90-9 119962-71-9  
RL: RCT (Reactant)  
(condensation of, with hydroxylysine deriv., in prepn. of bactericide)
- IT 15761-38-3, BOC-Ala-OH  
RL: RCT (Reactant)



(condensation of, with malonate)  
 IT 3850-40-6 4530-20-5 7764-95-6 15761-38-3 119962-72-0  
 RL: RCT (Reactant)  
 (condensation of, with .beta.-amino lysine deriv., in prepn. of bactericide)  
 IT 3262-72-4  
 RL: RCT (Reactant)  
 (condensation of, with .beta.-lysine deriv., in prepn. of bactericide)  
 IT 105-45-3, Methyl acetoacetate  
 RL: PROC (Process)  
 (conversion of, to silyl enol ether)  
 IT 111408-79-8  
 RL: RCT (Reactant)  
 (hydrogenation of, in prepn. of bactericide)  
 IT 111337-84-9 111337-85-0 111337-86-1 111465-40-8  
 RL: RCT (Reactant)  
 (manuf. with Pseudomonas fluorescens, in synthesis of bactericides)  
 IT 74-88-4, Methyl iodide, reactions  
 RL: RCT (Reactant)  
 (methylation of, of hydroxylysine deriv., in prepn. of bactericide)  
 IT 119962-69-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and condensation of, with aminopimelic acid deriv.)  
 IT 67609-52-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and cyclocondensation of, with alaninal deriv., in prepn. of bactericide)  
 IT 119960-28-0P 119960-29-1P 119960-30-4P 119960-31-5P 119960-32-6P  
 119960-33-7P 119960-34-8P 119960-35-9P 119960-36-0P 119960-37-1P  
 119960-38-2P 119960-39-3P 119960-40-6P 119960-41-7P 119960-42-8P  
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 119960-48-4P 119960-49-5P 119960-50-8P **119960-51-9P**  
 119960-52-0P 119960-53-1P 119960-54-2P 119960-55-3P 119960-56-4P  
 119960-57-5P 119960-58-6P 119960-59-7P 119960-60-0P 119960-61-1P  
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 120053-43-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and deprotection of, in prepn. of bactericide)  
 IT 119962-97-9P 119962-98-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and deprotection of, in prepn. of hydroxylysine bactericide)  
 IT 111305-50-1P 119960-62-2P 119960-63-3P 119960-64-4P 119960-65-5P  
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, in prepn. of bactericide)

IT 119962-89-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of, in prepn. of hydroxylysine bactericide)

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119962-50-4P 119962-51-5P 119962-52-6P 119962-54-8P 119962-55-9P  
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119976-74-8P 119976-75-9P 119976-76-0P 119976-77-1P 119976-78-2P  
119976-79-3P 119976-80-6P 119976-81-7P 119976-82-8P 119976-83-9P  
119976-84-0P 119976-85-1P 119976-86-2P 119976-87-3P 119976-88-4P  
119976-89-5P 119976-90-8P 119976-94-2P 120021-46-7P 120021-47-8P  
120021-48-9P 120021-49-0P 120021-50-3P 120021-51-4P 120021-52-5P  
120021-53-6P 120021-54-7P 120053-44-3P 120053-45-4P 120053-46-5P

RL: BAC (Biological activity or effector, except adverse); SPN  
(Synthetic preparation); BIOL (Biological study); PREP  
(Preparation)

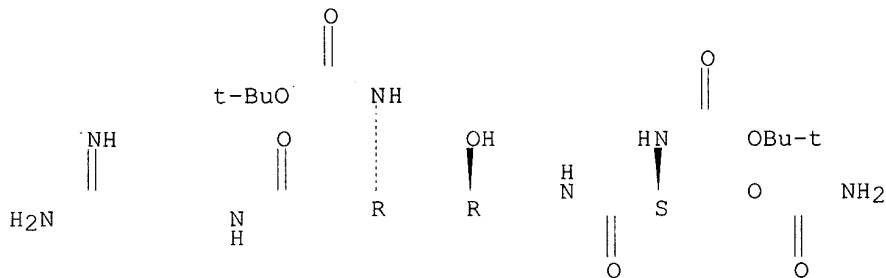
(prepn. of, as bactericide)

IT 7013-07-2P 62269-44-7P 80503-94-2P 82961-77-1P 87554-49-2P  
101669-78-7P 109579-16-0P 111305-59-0P 111305-61-4P 111305-62-5P  
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119962-88-8P 119962-93-5P 119962-95-7P 119962-99-1P 119976-92-0P  
120021-29-6P 120021-30-9P 120021-31-0P 120021-32-1P 120021-33-2P  
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120021-39-8P 120052-38-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

- (prepn. of, as bactericide intermediate)
- IT 119963-01-8P 119963-02-9P 119963-03-0P 119963-04-1P 119963-05-2P  
120021-57-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)
- (prepn. of, as intermediate for bactericide)
- IT 107-30-2, Methoxymethyl chloride 116-11-0 994-30-9, Triethylsilyl  
chloride 3970-21-6, Methoxyethoxymethyl chloride 25512-65-6,  
Dihydropyran 58479-61-1, tert-Butyldiphenylsilyl chloride  
RL: RCT (Reactant)
- (protection by, of hydroxylysine deriv., in prepn. of bactericide)
- IT 111305-66-9 111305-70-5 111337-87-2 119962-92-4 119962-94-6  
120021-56-9  
RL: RCT (Reactant)
- (reaction of, in prepn. of bactericide)
- IT 867-44-7 34670-47-8, 1-Methylhydrazinoacetic acid 51127-12-9  
119976-93-1  
RL: RCT (Reactant)
- (reaction of, in prepn. of hydroxylysine bactericide)
- IT 75-77-4, Trimethylsilyl chloride, reactions 2986-19-8,  
S-Methylisothiouraea 22509-74-6, N-Carboethoxyphthalimide  
RL: RCT (Reactant)
- (reaction of, with hydroxylysine deriv., in prepn. of bactericide)
- IT 86-81-7, 3,4,5-Trimethoxybenzaldehyde  
RL: RCT (Reactant)
- (reductive alkylation by, of hydroxylysine deriv., in prepn. of  
bactericide)
- IT 100-52-7, Benzaldehyde, reactions  
RL: RCT (Reactant)
- (reductive alkylation by, of hydroxylysine deriv., in prepn. of sodium  
cyanoborohydride)
- IT 75-07-0, Acetaldehyde, reactions  
RL: RCT (Reactant)
- (reductive ethylation by, of amino acid deriv., in presence of sodium  
cyanoborohydride)
- IT 50-00-0, Formaldehyde, reactions  
RL: RCT (Reactant)
- (reductive methylation of amino acid by, in the presence of sodium  
cyanoborohydride)
- IT 110-60-1, 1,4-Butanediamine  
RL: RCT (Reactant)
- (ring-opening by, of .delta.-lactone)
- IT 119960-51-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)
- (prepn. and deprotection of, in prepn. of bactericide)
- RN 119960-51-9 HCAPLUS  
CN L-threo-Hexonamide, 6-[[3-[(aminocarbonyl)oxy]-2-[[[(1,1-  
dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]-N-(3-amino-3-  
iminopropyl)-2,3,4,6-tetradecoxy-3-[[[(1,1-dimethylethoxy)carbonyl]amino]-,  
monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

IT 119961-60-3P

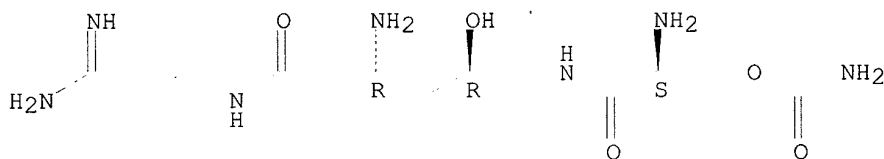
RL: BAC (Biological activity or effector, except adverse); **SPN**  
**(Synthetic preparation)**; BIOL (Biological study); **PREP**  
**(Preparation)**

(prepn. of, as bactericide)

RN 119961-60-3 HCAPLUS

CN L-threo-Hexonamide, 3-amino-6-[[2-amino-3-[(aminocarbonyl)oxy]-1-oxopropyl]amino]-N-(3-amino-3-iminopropyl)-2,3,4,6-tetradecoxy-, trihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●3 HCl

L33 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1972:419419 HCAPLUS

DN 77:19419

TI Chloroformate and carbonate derivatives of substituted and unsubstituted  
 1-phenyl-2,2-dialkyl-1,3-dihydroxypropanes

IN Kulka, Kurt

PA Fritzsche Dodge and Olcott Inc.

SO U.S., 10 pp. Division of U.S. 3,415,844 (CA 71:91102q).

CODEN: USXXAM

DT Patent

LA English

IC C07C; A61K

NCL 260463000

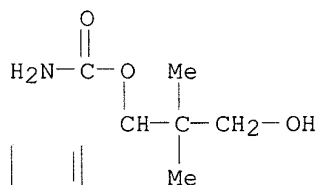
CC 25-21 (Noncondensed Aromatic Compounds)

FAN.CNT 1

| PATENT NO. | KIND | DATE  | APPLICATION NO. | DATE  |
|------------|------|-------|-----------------|-------|
| -----      | ---- | ----- | -----           | ----- |

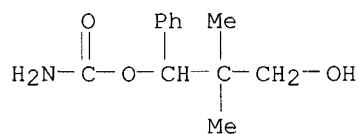
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PI US 3629314 A 19711221 US 1968-761875 19680923  
 GI For diagram(s), see printed CA Issue.  
 AB Monocarbamates (I) (R = H, OMe, Me<sub>2</sub>CH, Me, Cl; R<sub>1</sub> = H or RR<sub>1</sub> = OCH<sub>2</sub>O; R<sub>2</sub> = H or CONH<sub>2</sub> .noteq. R<sub>3</sub> = H or CONH<sub>2</sub>) were prepd. from the corresponding propanediols by treatment with ClCO<sub>2</sub>R (R = Et or Me) and Me<sub>3</sub>N to give the corresponding monoalkyl and **cyclic** carbonates and then **ammonolysis** of the carbonates. The monocarbamates were potential tranquilizers.  
 ST carbamate tranquilizer; propanediol carbamate tranquilizer  
 IT 24020-78-8P **24020-79-9P** 24020-80-2P 24020-81-3P  
 24020-82-4P 24020-83-5P 24020-84-6P 24020-85-7P 24020-86-8P  
 24020-87-9P 24020-88-0P 24020-89-1P 24020-90-4P 24020-91-5P  
 24026-62-8P 24026-65-1P **24026-66-2P** **24026-67-3P**  
 24026-70-8P 24026-75-3P **24026-76-4P** 24063-46-5P  
 35615-31-7P 36088-40-1P 36088-41-2P 36088-42-3P 36088-43-4P  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (prepn. of)  
 IT 33950-46-8  
 RL: RCT (Reactant)  
 (reaction of with phosgene)  
 IT 79-22-1  
 RL: RCT (Reactant)  
 (reaction of, with (methoxyphenyl)dimethyldihydroxypropane)  
 IT 103-71-9  
 RL: RCT (Reactant)  
 (reaction of, with (methylenedioxy)phenyl-2,2-dimethyldihydroxypropane)  
 IT 24793-94-0 35615-33-9  
 RL: RCT (Reactant)  
 (reaction of, with ethyl chloroformate)  
 IT 35613-25-3  
 RL: RCT (Reactant)  
 (reaction of, with ethyl isocyanate)  
 IT 35615-32-8  
 RL: RCT (Reactant)  
 (reaction of, with ethylchloroformate)  
 IT 24793-83-7  
 RL: RCT (Reactant)  
 (reaction of, with methyl chloroformate)  
 IT 109-90-0  
 RL: RCT (Reactant)  
 (reaction of, with naphthyldimethyldihydroxypropane)  
 IT 75-44-5  
 RL: RCT (Reactant)  
 (reaction of, with phenyldimethyldihydroxypropane)  
 IT 31758-87-9  
 RL: RCT (Reactant)  
 (reaction of, with phosgene)  
 IT **24020-79-9P** **24026-66-2P** **24026-67-3P**  
**24026-76-4P**  
 RL: **SPN (Synthetic preparation); PREP (Preparation)**  
 (prepn. of)  
 RN 24020-79-9 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)

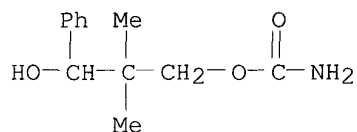


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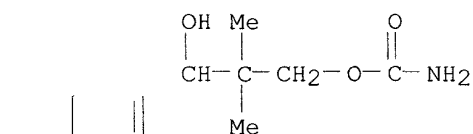
RN 24026-66-2 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-67-3 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-76-4 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



Cl

L33 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1972:405217 HCAPLUS  
 DN 77:5217  
 TI Monocarbamates and n-alkyl or N-phenyl monocarbamates of substituted and unsubstituted 1-phenyl-2,2-dialkyl-1,3-dihydroxypropanes  
 IN Kulka, Kurt  
 PA Fritzsche Dodge and Olcott Inc.  
 SO U.S., 11 pp. Division of U.S. 3,415,844 (CA 71:91102q).  
 CODEN: USXXAM

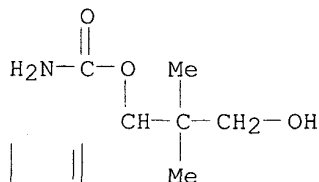
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DT Patent  
 LA English  
 IC C07D  
 NCL 260340500  
 CC 25-21 (Noncondensed Aromatic Compounds)  
 Section cross-reference(s): 28

FAN.CNT 1

|    | PATENT NO.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | KIND        | DATE        | APPLICATION NO. | DATE              |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-------------|-----------------|-------------------|
| PI | US 3637753                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | A           | 19720125    | US 1968-761797  | 19680923          |
| GI | For diagram(s), see printed CA Issue.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |             |             |                 |                   |
| AB | Division of U.S. 3,415,844 (CA 71: 91102q). The title compds., useful animal relaxants, were prepd. Thus, 1-(4-methoxyphenyl)-2,2-dimethyl-1,3-dihydroxypropane (I), MeO <sub>2</sub> CCl, pyridine, and C <sub>6</sub> H <sub>6</sub> was stirred 1 hr and then heated 5 hr at 52-62.degree. to give 15-20% of the <b>cyclic</b> carbonate (II, R = 4-MeO) of I. <b>NH<sub>3</sub></b> (g) was passed 17 hr into a soln. of II in aq. <b>NH<sub>3</sub></b> -isopropanol to give a mixt. of mono carbamates RC <sub>6</sub> H <sub>4</sub> CH(O <sub>2</sub> CNHR <sub>1</sub> )CMe <sub>2</sub> CH <sub>2</sub> OH (III, R = 4-MeO, R <sub>1</sub> = H) and RC <sub>6</sub> H <sub>4</sub> CH(OH)CMe <sub>2</sub> CH <sub>2</sub> O <sub>2</sub> CNHR <sub>1</sub> (IV, R = 4-MeO, R <sub>1</sub> = H). Similarly prepd. were .apprx.10 analogs of II as well as .apprx.10 carbamate mixts. including III (R = H, R <sub>1</sub> = Ph) and IV (R = H, R <sub>1</sub> = Ph). |             |             |                 |                   |
| ST | carbamate phenyl hydroxypropane; carbonate phenyl hydroxypropane                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |             |             |                 |                   |
| IT | 24020-78-8P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24020-79-9P | 24020-80-2P | 24020-81-3P     |                   |
|    | 24020-82-4P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24020-83-5P | 24020-84-6P | 24020-90-4P     | 24020-91-5P       |
|    | 24020-92-6P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24020-93-7P | 24026-60-6P | 24026-61-7P     | 24026-62-8P       |
|    | 24026-63-9P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-64-0P | 24026-65-1P |                 |                   |
|    | 24026-66-2P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-67-3P | 24026-68-4P | 24026-69-5P     |                   |
|    | 24026-70-8P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-71-9P | 24026-72-0P | 24026-73-1P     |                   |
|    | 24026-74-2P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-75-3P | 24026-76-4P | 24026-77-5P     |                   |
|    | 24026-78-6P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24063-00-1P | 24063-01-2P | 24793-83-7P     |                   |
|    | 24793-94-0P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 25321-45-3P | 25321-46-4P | 25321-47-5P     | 25321-48-6P       |
|    | 25321-49-7P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 25897-12-5P | 36851-20-4P | 36851-21-5P     |                   |
|    | 36851-22-6P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 36851-23-7P | 36911-07-6P | 36911-08-7P     |                   |
|    | RL: <b>SPN (Synthetic preparation); PREP (Preparation)</b><br>(prepn. of)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |             |             |                 |                   |
| IT | 36851-29-3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |             |             |                 |                   |
|    | RL: RCT (Reactant)<br>(reaction of, with <b>ammonia</b> and phosgene)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |             |             |                 |                   |
| IT | 78-84-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |             |             |                 |                   |
|    | RL: RCT (Reactant)<br>(reaction of, with benzaldehydes)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |             |             |                 |                   |
| IT | 31758-87-9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 33950-46-8  | 35613-25-3  | 35615-33-9      | 36851-35-1        |
|    | RL: RCT (Reactant)<br>(reaction of, with chloroformates)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |             |             |                 |                   |
| IT | 122-03-2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 123-11-5    | 1334-78-7   |                 |                   |
|    | RL: RCT (Reactant)<br>(reaction of, with isobutyraldehyde)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |             |             |                 |                   |
| IT | 75-44-5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 79-22-1     | 103-71-9    | 109-90-0        | 541-41-3 624-83-9 |
|    | RL: RCT (Reactant)<br>(reaction of, with phenyldihydroxypropanes)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |             |             |                 |                   |
| IT | <b>7664-41-7</b> , reactions                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |             |             |                 |                   |
|    | RL: RCT (Reactant)<br>(with carbonate and formate esters)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |             |             |                 |                   |
| IT | 24020-79-9P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-63-9P | 24026-64-0P |                 |                   |
|    | 24026-66-2P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-67-3P | 24026-71-9P |                 |                   |
|    | 24026-72-0P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 24026-76-4P | 24063-00-1P |                 |                   |
|    | 24063-01-2P                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 25321-48-6P | 25321-49-7P |                 |                   |
|    | RL: <b>SPN (Synthetic preparation); PREP (Preparation)</b><br>(prepn. of)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |             |             |                 |                   |
| RN | 24020-79-9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | HCAPLUS     |             |                 |                   |

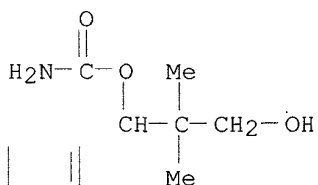
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



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RN 24026-63-9 HCAPLUS

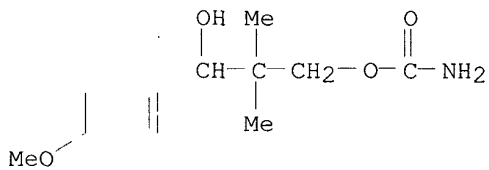
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



MeO

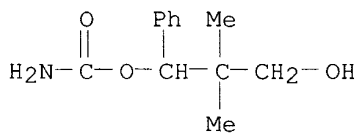
RN 24026-64-0 HCAPLUS

CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



RN 24026-66-2 HCAPLUS

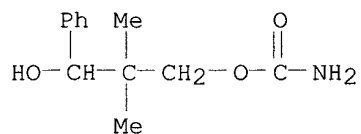
CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



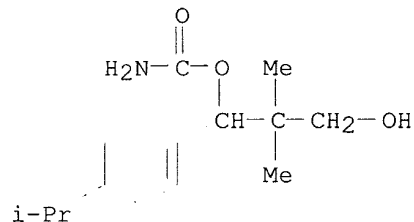
RN 24026-67-3 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)

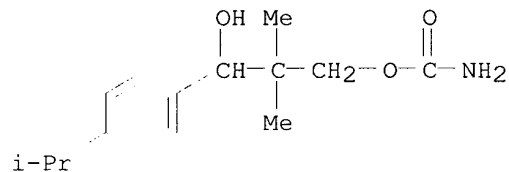




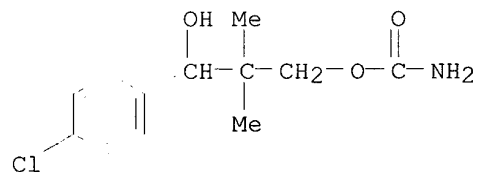
RN 24026-71-9 HCAPLUS  
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate  
(9CI) (CA INDEX NAME)



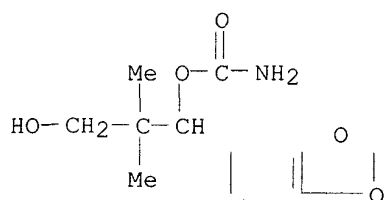
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CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 3-carbamate  
(9CI) (CA INDEX NAME)



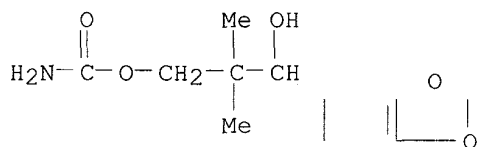
RN 24026-76-4 HCAPLUS  
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



RN 24063-00-1 HCAPLUS  
CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI)  
(CA INDEX NAME)



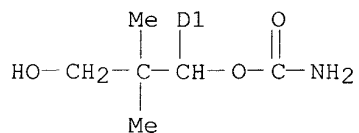
RN 24063-01-2 HCAPLUS  
 CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 3-carbamate (9CI)  
 (CA INDEX NAME)



RN 25321-48-6 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 1-carbamate (9CI) (CA  
 INDEX NAME)



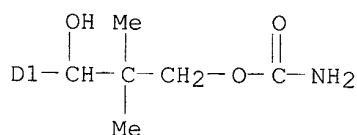
D1-Me



RN 25321-49-7 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA  
 INDEX NAME)



D1-Me



IT 7664-41-7, reactions  
 RL: RCT (Reactant)  
 (with carbonate and formate esters)  
 RN 7664-41-7 HCAPLUS  
 CN Ammonia (8CI, 9CI) (CA INDEX NAME)

NH<sub>3</sub>

L33 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1970:21476 HCAPLUS  
 DN 72:21476  
 TI Hypnotic and tranquilizing 1-aryl-2,2-dialkyl-1,3-dihydroxypropane derivatives  
 IN Kulka, Kurt  
 PA Fritzsche Brothers, Inc.  
 SO S. African, 46 pp.  
 CODEN: SFXXAB  
 DT Patent  
 LA English  
 CC 25 (Noncondensed Aromatic Compounds)  
 FAN.CNT 1

|    | PATENT NO. | KIND | DATE     | APPLICATION NO. | DATE     |
|----|------------|------|----------|-----------------|----------|
| PI | ZA 6704670 |      | 19690203 | ZA              | 19670803 |

GI For diagram(s), see printed CA Issue.  
 AB p-R1C6H4CH(OR2)CMeRCH2OR3 (I) and II (R = Me or Pr, R1 = H, Me, MeO, iso-Pr, or Cl, R2 and R3 = H, CO2Me, CO2Et, CONH2, CONHMe, CONHEt, or CONHPh), having sedative, hypnotic, and tranquilizing activities are prepd. from I (R2 = R3 = H). For example, 140 g 85% methanolic KOH was treated with a mixt. of 272 g p-MeOC6H4CHO and 360 g iso-PrCHO over 1.5 hr at 44-9.degree., stirred at 42.degree. for 3 hr, cooled to 30.degree., acidified (AcOH), concd. to remove 250 ml MeOH, and dild. with water to sep. 65.5% I (R = Me, R1 = MeO, R2 = R3 = H) (III), b6 178-93.degree., m. 71.5-2.degree.. A mixt. of 50 g III, 70 ml benzene, and 26 g pyridine was treated with 37 g ClCO2Me in 30 ml benzene at 18-25.degree. over 45 min, stirred at room temp. and 52-62.degree. for 1 and 5 hr, resp. to give a mixt. of monomethyl and cyclic carbonates of III. II (R = Me, R1 = MeO, 15-20%), m. 138-9.degree., was crystd. from iso-PrOH. Introduction of NH<sub>3</sub> into a mixt. of 55 g III, 80 ml iso-PrOH and

30 ml 28% aq. **NH3** at room temp. for 17 hr gave 50 g monocarbamate mixt. of III. A soln. of 218 g COCl<sub>2</sub> in 2 l. toluene was treated with 180 g I (R = Me, R<sub>1</sub> = R<sub>2</sub> = R<sub>3</sub> = H) (IV) in 100 g pyridine and 500 ml CHCl<sub>3</sub> at -1-4.degree. over 12.5 hr to give, after 17 hr, 90% II (R = Me, R<sub>1</sub> = H) (V), m. 112-14.degree.. Treatment of V with **NH3** gave 54.2% monocarbamate mixt. of IV. A soln. of 214 g I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = R<sub>3</sub> = H) (VI) in 400 ml tetrahydrofuran contg. 125 g PhNMe<sub>2</sub> was added to 104 g COCl<sub>2</sub> in 200 ml toluene at -5.degree., cooled to -7.degree., treated with 2 moles 28-9% aq. **NH3** to give, after removal of PhNMe<sub>2</sub> by steam distn., 50-5% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = H, R<sub>3</sub> = CONH<sub>2</sub>), m. 134.degree.. Treatment of 0.5 mole VI and 0.54 mole Et<sub>3</sub>N in 150 ml benzene with 0.55 mole ClCO<sub>2</sub>Et gave 137.5 g monoethyl carbonate mixt. of VI, which was heated at 120-70.degree./6-7 mm for 20 hr to give 82.1 g II (R = Me, R<sub>1</sub> = Cl,) (VII), m. 120-3.degree.. Treatment of 240 g VII in 360 ml iso-PrOH contg. 100 ml 28-9% aq. **NH3** with **NH3** for 18 hr at 35-40.degree. gave 45% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = CONH<sub>2</sub>, R<sub>3</sub> = H), m. 171.degree.. A soln. of 180 g IV in 200 ml tetrahydrofuran was treated with a soln. of 62.7 g MeNCO in 100 ml tetrahydrofuran followed by 3 drops pyridine to give, after 24 hr 70% monomethylcarbamate mixt. of IV. Acetylation of 53.6 g VI with 16.5 g AcOH in 150 ml toluene contg. 0.25 g p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H gave 80% I (R = Me, R<sub>1</sub> = Cl, R<sub>2</sub> = H, R<sub>3</sub> = Ac), m. 78.5-80.degree.. Treatment of I (R = Me, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Ac) (VIII) and Et<sub>3</sub>N in toluene with COCl<sub>2</sub> followed by **NH3** and subsequent hydrolysis gave I (R = Me, R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = CONH<sub>2</sub>). Treatment of VIII and Et<sub>3</sub>N in toluene with ClCO<sub>2</sub>Et followed by **NH3** and subsequent hydrolysis gave I (R = Me, R<sub>1</sub> = R<sub>3</sub> = H, R<sub>2</sub> = CONH<sub>2</sub>). Other compds. such as derivs. of 1-(3,4-methylenedioxyphenyl)- and 1-(1-naphthyl)-2,2-dimethyl-1,3-dihydroxypropanes are also similarly prepd.

ST benzenes dihydroxypropyl substituted; hypnotic dihydroxypropylbenzenes; dihydroxypropylbenzenes hypnotic; tranquilizers dihydroxypropylbenzenes

IT 24020-78-8P 24020-79-9P 24020-80-2P 24020-81-3P  
24020-82-4P 24020-83-5P 24020-84-6P 24020-85-7P 24020-86-8P  
24020-87-9P 24020-88-0P 24020-89-1P 24020-90-4P 24020-91-5P  
24020-92-6P 24020-93-7P 24026-60-6P 24026-61-7P 24026-62-8P  
24026-63-9P 24026-64-0P 24026-65-1P  
24026-66-2P 24026-67-3P 24026-68-4P 24026-69-5P  
24026-70-8P 24026-71-9P 24026-72-0P 24026-73-1P  
24026-74-2P 24026-75-3P 24026-76-4P 24026-77-5P  
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25321-48-6P 25321-49-7P 25897-12-5P

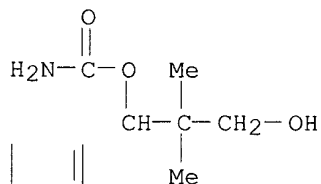
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(prepn. of)

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24026-72-0P 24026-76-4P 24063-00-1P 24063  
-01-2P 25321-48-6P 25321-49-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 24020-79-9 HCAPLUS

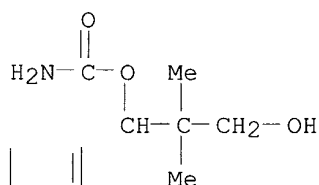
CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA  
INDEX NAME)



Cl

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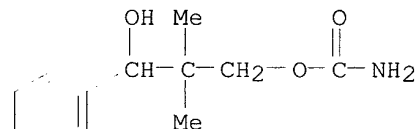
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MeO

RN 24026-64-0 HCAPLUS

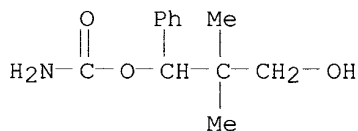
CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



MeO

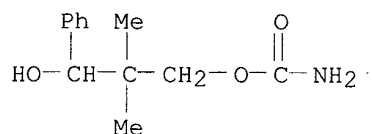
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CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)

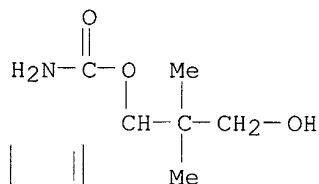


RN 24026-67-3 HCAPLUS

CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)

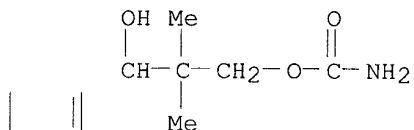


RN 24026-71-9 HCAPLUS  
CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate  
(9CI) (CA INDEX NAME)



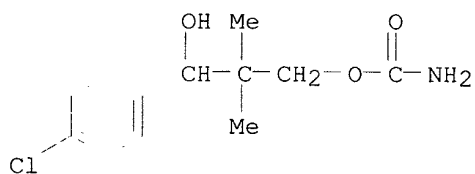
i-Pr

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(9CI) (CA INDEX NAME)

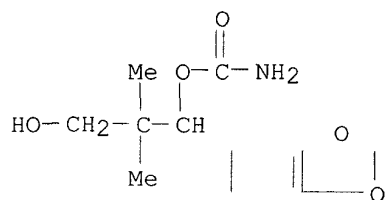


i-Pr

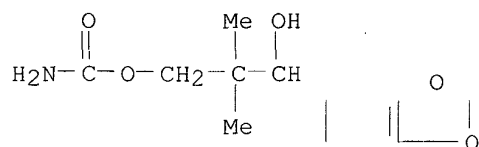
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CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)



RN 24063-00-1 HCAPLUS  
CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI)  
(CA INDEX NAME)



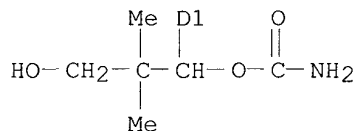
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RN 25321-48-6 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 1-carbamate (9CI) (CA INDEX NAME)

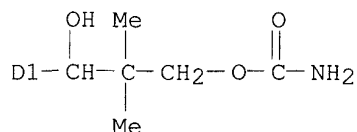


D1--Me



RN 25321-49-7 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA INDEX NAME)

D1-Me

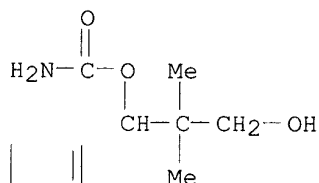


L33 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1969:491101 HCAPLUS  
 DN 71:91101  
 TI Derivatives of glycol carbonates and carbamates  
 PA Fritzsche Brothers, Inc.  
 SO Fr., 16 pp.  
 CODEN: FRXXAK  
 DT Patent  
 LA French  
 IC C07C; A61K  
 CC 25 (Noncondensed Aromatic Compounds)  
 FAN.CNT 1

|    | PATENT NO.                                                                                                                                                                                                                                                                    | KIND        | DATE        | APPLICATION NO. | DATE        |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------|-------------|-----------------|-------------|
| PI | FR 1534503                                                                                                                                                                                                                                                                    |             | 19680726    | FR              | 19670821    |
| AB | 1-Phenyl-2,2-dialkyl-1,3-dihydroxypropanes, and their derivs, substituted in the C6H6 ring, were converted into carbonates, carbamates and N-substituted carbamates. Thus, 4-ClC6H4CH(OH)CMe2CH2OH, treated successively with COCl2 and NH3 gave 4-ClC6H4CH(OH)CMe2CH2OCONH2. |             |             |                 |             |
| ST | carbonates glycol; glycol carbonates; carbamates glycol                                                                                                                                                                                                                       |             |             |                 |             |
| IT | 24020-78-8P                                                                                                                                                                                                                                                                   | 24020-79-9P | 24020-80-2P | 24020-81-3P     |             |
|    | 24020-82-4P                                                                                                                                                                                                                                                                   | 24020-83-5P | 24020-84-6P | 24020-85-7P     | 24020-86-8P |
|    | 24020-87-9P                                                                                                                                                                                                                                                                   | 24020-88-0P | 24020-89-1P | 24020-90-4P     | 24020-91-5P |
|    | 24020-92-6P                                                                                                                                                                                                                                                                   | 24020-93-7P | 24026-60-6P | 24026-61-7P     | 24026-62-8P |
|    | 24026-63-9P                                                                                                                                                                                                                                                                   | 24026-64-0P | 24026-65-1P |                 |             |
|    | 24026-66-2P                                                                                                                                                                                                                                                                   | 24026-67-3P | 24026-68-4P | 24026-69-5P     |             |
|    | 24026-70-8P                                                                                                                                                                                                                                                                   | 24026-71-9P | 24026-72-0P | 24026-73-1P     |             |
|    | 24026-74-2P                                                                                                                                                                                                                                                                   | 24026-75-3P | 24026-76-4P | 24026-77-5P     |             |
|    | 24026-78-6P                                                                                                                                                                                                                                                                   | 24063-00-1P | 24063-01-2P | 24063-46-5P     |             |
|    | 25321-45-3P                                                                                                                                                                                                                                                                   | 25321-46-4P | 25321-47-5P | 25321-48-6P     |             |
|    | 25321-49-7P                                                                                                                                                                                                                                                                   |             |             |                 |             |
|    | RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)                                                                                                                                                                                                               |             |             |                 |             |
| IT | 24020-79-9P                                                                                                                                                                                                                                                                   | 24026-63-9P | 24026-64-0P |                 |             |
|    | 24026-66-2P                                                                                                                                                                                                                                                                   | 24026-67-3P | 24026-71-9P |                 |             |
|    | 24026-72-0P                                                                                                                                                                                                                                                                   | 24026-76-4P | 24063-00-1P |                 |             |
|    | 24063-01-2P                                                                                                                                                                                                                                                                   | 25321-48-6P | 25321-49-7P |                 |             |
|    | RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)                                                                                                                                                                                                               |             |             |                 |             |
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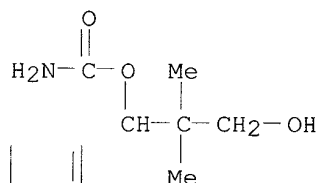


CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)



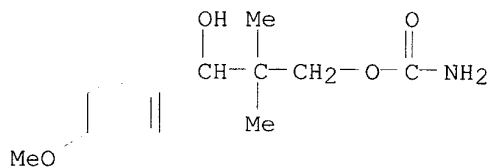
Cl

RN 24026-63-9 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-methoxyphenyl)-2,2-dimethyl-, 1-carbamate (9CI) (CA INDEX NAME)

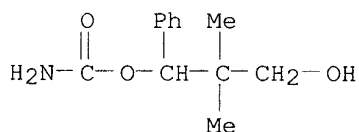


MeO

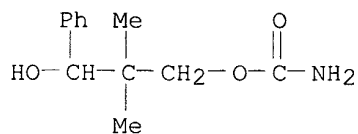
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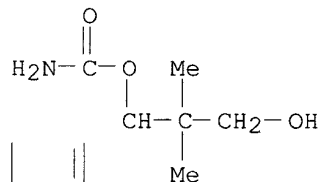
RN 24026-66-2 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 1-carbamate (8CI, 9CI) (CA INDEX NAME)



RN 24026-67-3 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-phenyl-, 3-carbamate (8CI, 9CI) (CA INDEX NAME)

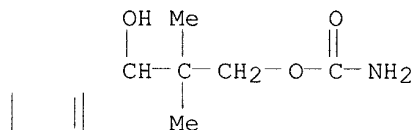


RN 24026-71-9 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 1-carbamate  
 (9CI) (CA INDEX NAME)



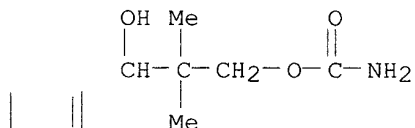
i-Pr

RN 24026-72-0 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-[4-(1-methylethyl)phenyl]-, 3-carbamate  
 (9CI) (CA INDEX NAME)



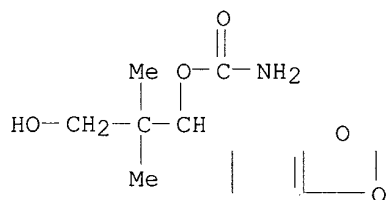
i-Pr

RN 24026-76-4 HCAPLUS  
 CN 1,3-Propanediol, 1-(4-chlorophenyl)-2,2-dimethyl-, 3-carbamate (9CI) (CA INDEX NAME)

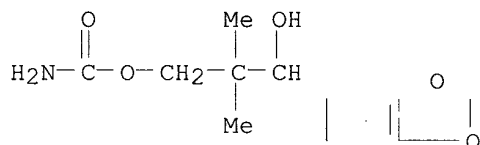


Cl

RN 24063-00-1 HCAPLUS  
 CN 1,3-Propanediol, 1-(1,3-benzodioxol-5-yl)-2,2-dimethyl-, 1-carbamate (9CI)  
 (CA INDEX NAME)



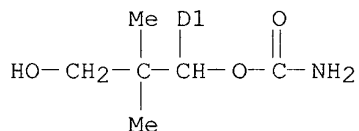
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 (CA INDEX NAME)



RN 25321-48-6 HCAPLUS  
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 INDEX NAME)

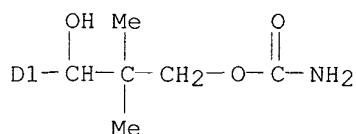


D1-Me



RN 25321-49-7 HCAPLUS  
 CN 1,3-Propanediol, 2,2-dimethyl-1-(methylphenyl)-, 3-carbamate (9CI) (CA  
 INDEX NAME)

D1-Me



L33 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2002 ACS

AN 1969:412494 HCAPLUS

DN 71:12494

TI Carbamate derivatives related to meprobamate

AU Ludwig, Bernard J.; Powell, Leo S.; Berger, Frank Milan

CS Wallace Lab., Carter-Wallace, Inc., Cranbury, N. J., USA

SO J. Med. Chem. (1969), 12(3), 462-72

CODEN: JMCMAR

DT Journal

LA English

CC 23 (Aliphatic Compounds)

AB A series of 2-substituted 1,3-propanediol dicarbamates, related chem. to meprobamate, was prepd. for central nervous system pharmacol. investigation. The N-unsubstituted propanediol dicarbamates were obtained by an ester-exchange reaction between the corresponding diol and urethane, by phosgenation of the diol followed by **ammoniation** of the bis(chlorocarbonate) deriv., by the reaction of the diol with cyanic acid, and by **ammoniation** of the bis(phenylcarbonate) deriv. of the appropriate diol. The sym. N,N'-substituted propanediol dicarbamates were synthesized by direct carbamoylation of the propanediols, and the unsym. substituted derivs. by stepwise carbamoylation via the m-dioxanone and hydroxypropyl carbamate intermediates using similar carbamoylation reactions. In addn. to the prepn. and phys. properties of these compds., the muscle paralyzing activity, anticonvulsant activity, and toxicity of these carbamates and many of the intermediates employed in their synthesis are presented. Structure-activity relations among these compds. are discussed.

ST propanediols carbamoylation; carbamoylation propanediols

IT Antispasmodics

IT Muscles, responses to chemicals  
(to propanediol carbamate derivs.)

IT 1,3-Propanediol, 2,2-diphenyl-, dicarbamate

1,3-Propanediol, 2-methyl-2-propyl-, bis(1-aziridinecarboxylate)

1,3-Propanediol, 2-sec-butyl-2-methyl-, carbamate carbazate (ester)

1-Aziridinecarboxylic acid, 2-methyl-2-propyltrimethylene ester

Carbazic acid, 2-(hydroxymethyl)-2,3-dimethylpentyl ester carbamate  
(ester)RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)IT 57-53-4P 64-55-1P 78-44-4P 1146-18-5P 1672-81-7P 1672-86-2P  
1729-14-2P 2037-62-9P 2109-29-7P 2109-30-0P 2109-88-8P

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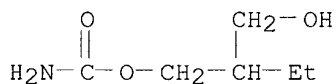
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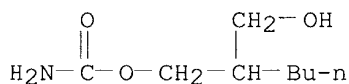
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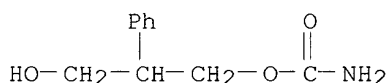
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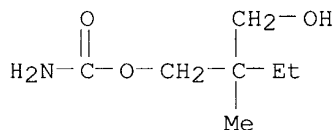
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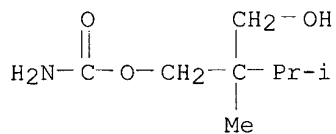
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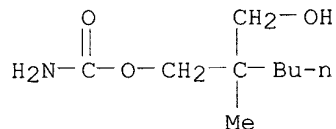


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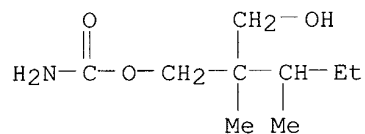
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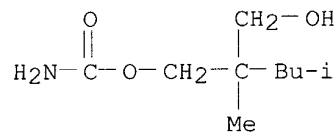
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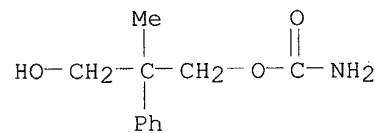
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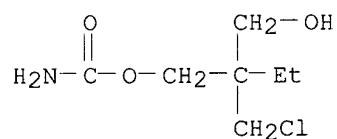
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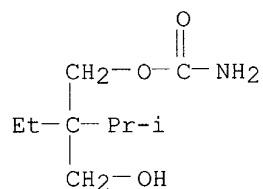
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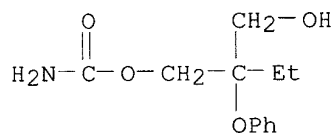
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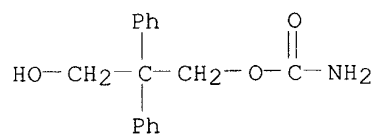
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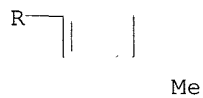
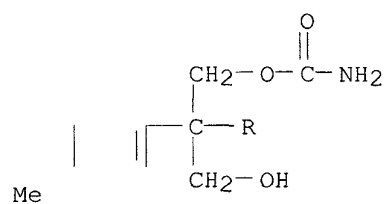


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CN 1,3-Propanediol, 2,2-di-p-tolyl-, monocarbamate (8CI) (CA INDEX NAME)





RN 25480-69-7 HCAPLUS  
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